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FIG.1

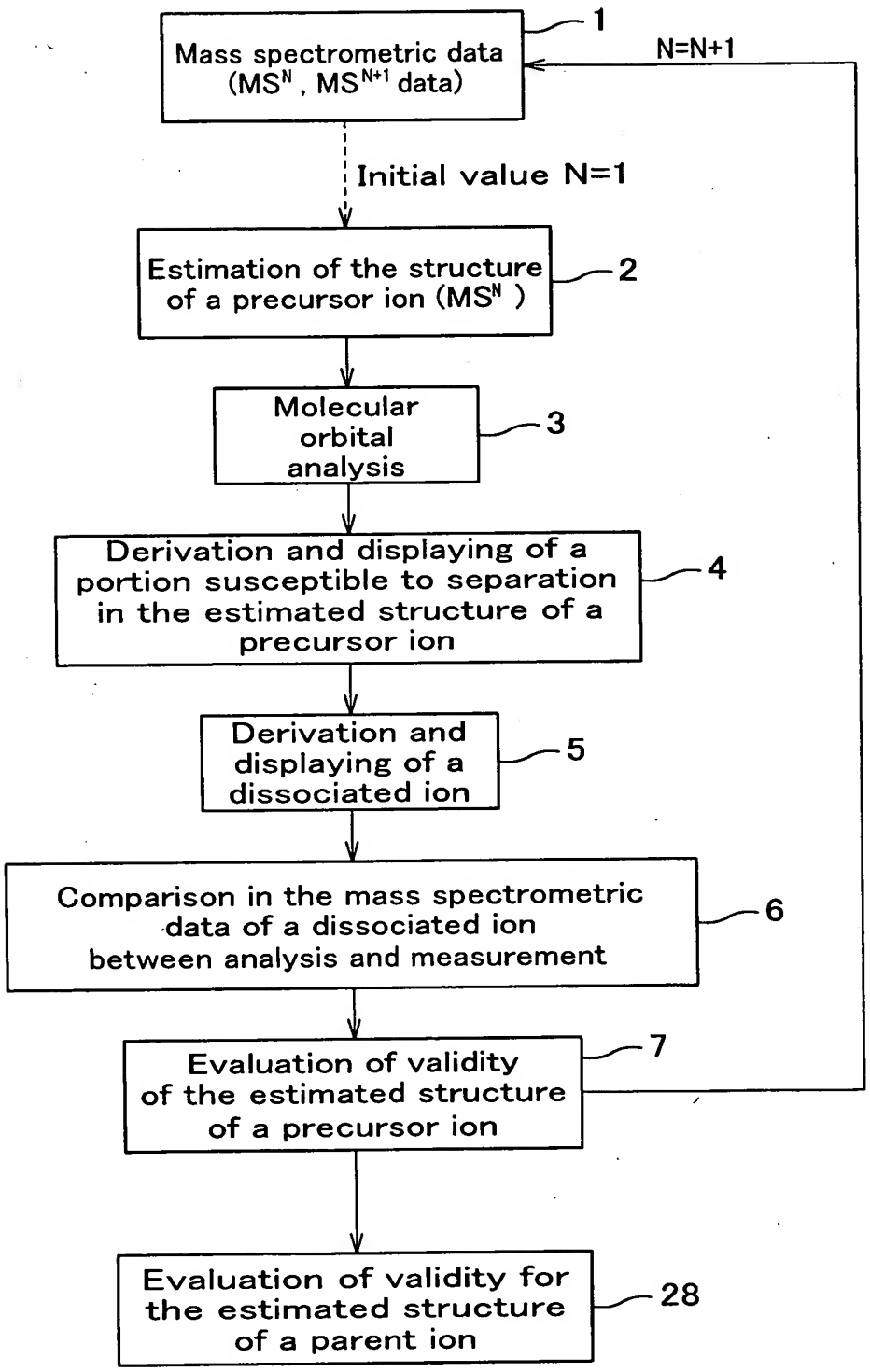

Mass spectrometric data (MS^N , MS^N+1 data)
1
N=N+1
Initial value N=1
Estimation of the structure of a precursor ion (MS^N)
2
Molecular orbital analysis
3
Derivation and displaying of a portion susceptible to separation in the estimated structure of a precursor ion
4
Derivation and displaying of a dissociated ion
5
Comparison in the mass spectrometric data of a dissociated ion between analysis and measurement
6
Evaluation of validity of the estimated structure of a precursor ion
7
Evaluation of validity for the estimated structure of a parent ion
28

FIG.2

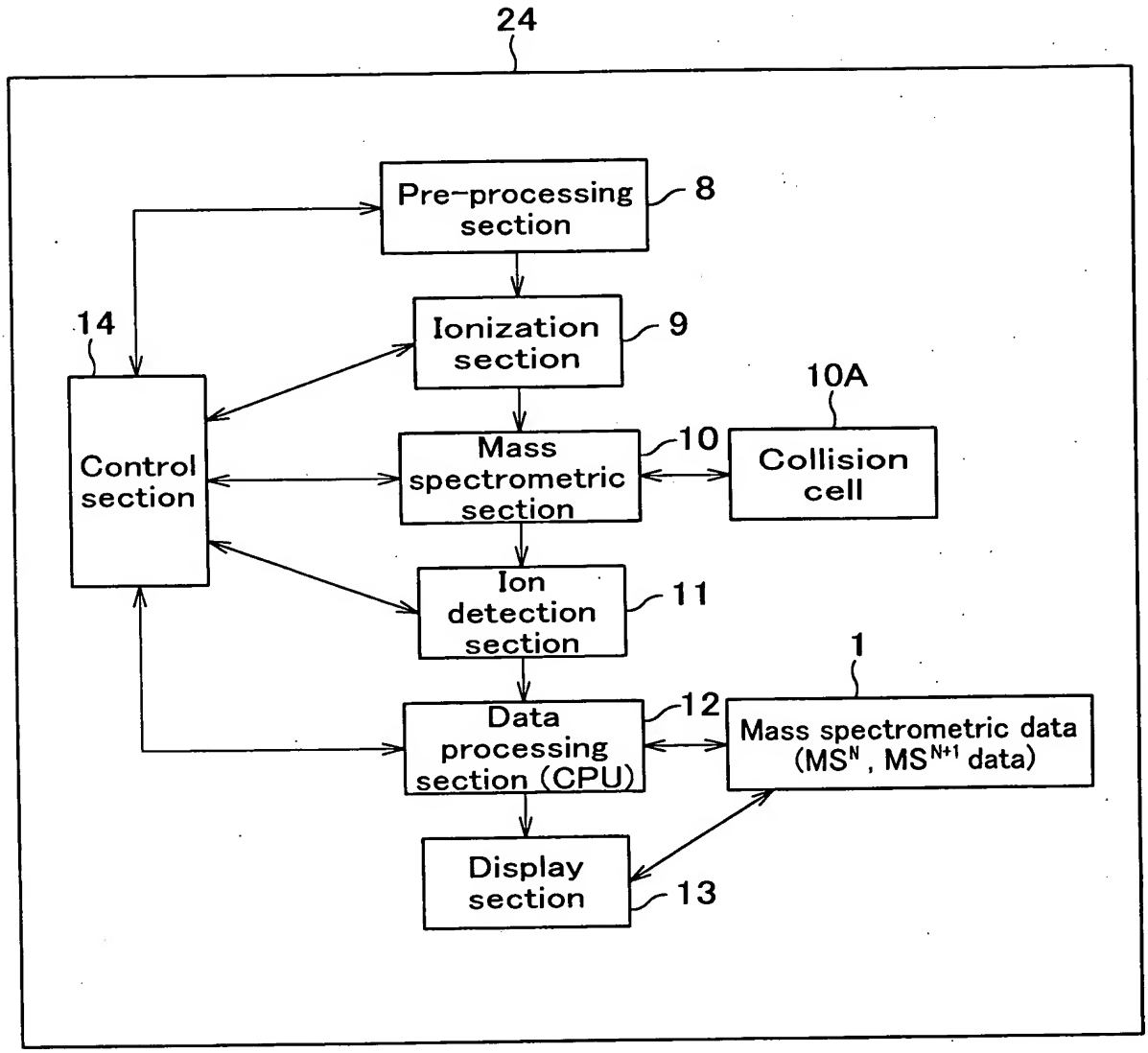

24
Pre-processing section
8
Ionization section
9
14
10A
Control section
Mass spectrometric section
10
Collision cell
Ion detection section
11
1
Data processing section (CPU)
12
Mass spectrometric data (MS^N, MS^N+1 data)
Display section
13

FIG.3

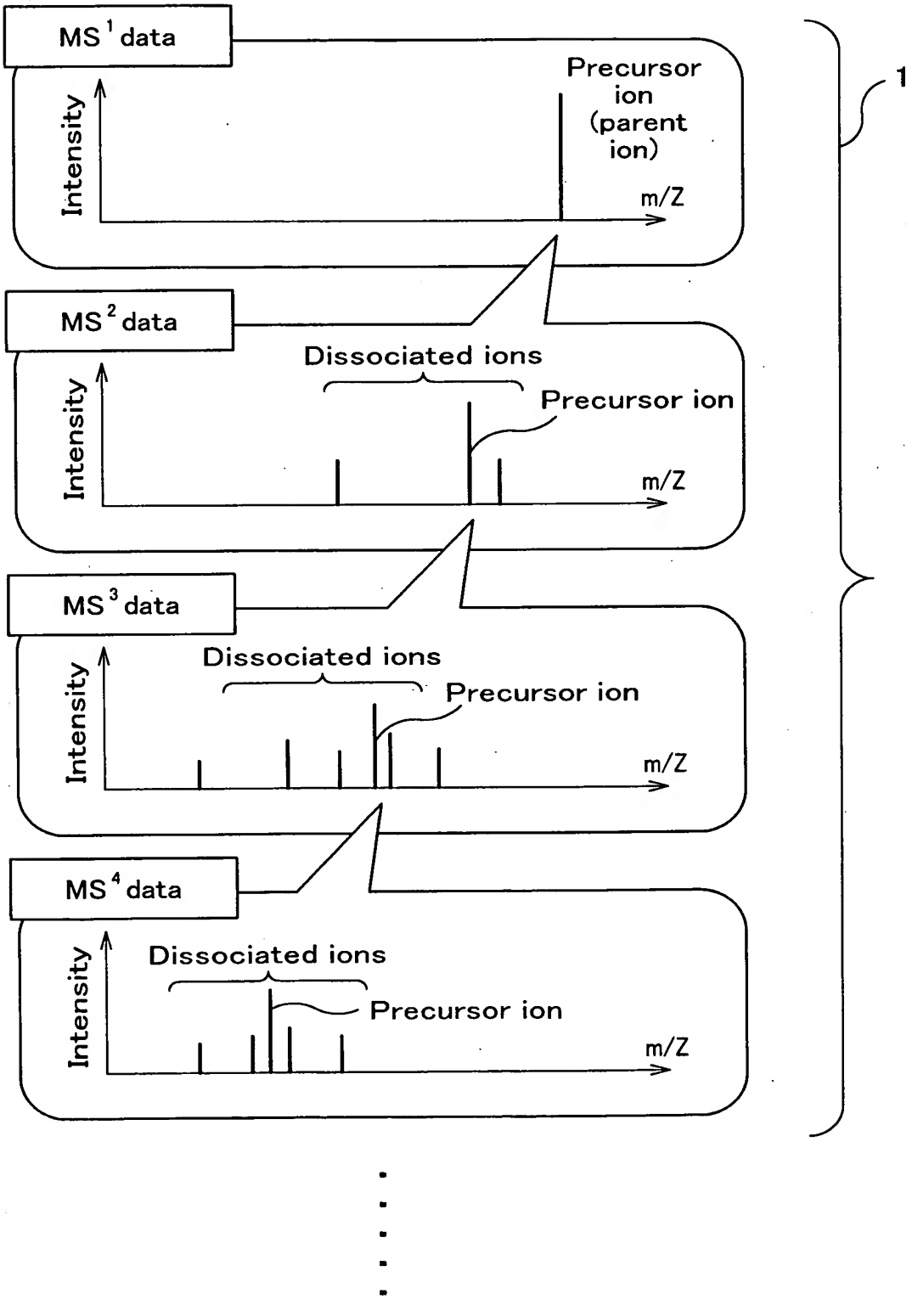

MS 1 data
Intensity
Precursor ion (parent ion)
m/Z
MS 2 data
Dissociated ions
Precursor ion
Intensity
m/Z
MS 3 data
Dissociated ions
Precursor ion
Intensity
m/Z
MS 4 data
Dissociated ions
Precursor ion
Intensity
m/Z
1

FIG.4

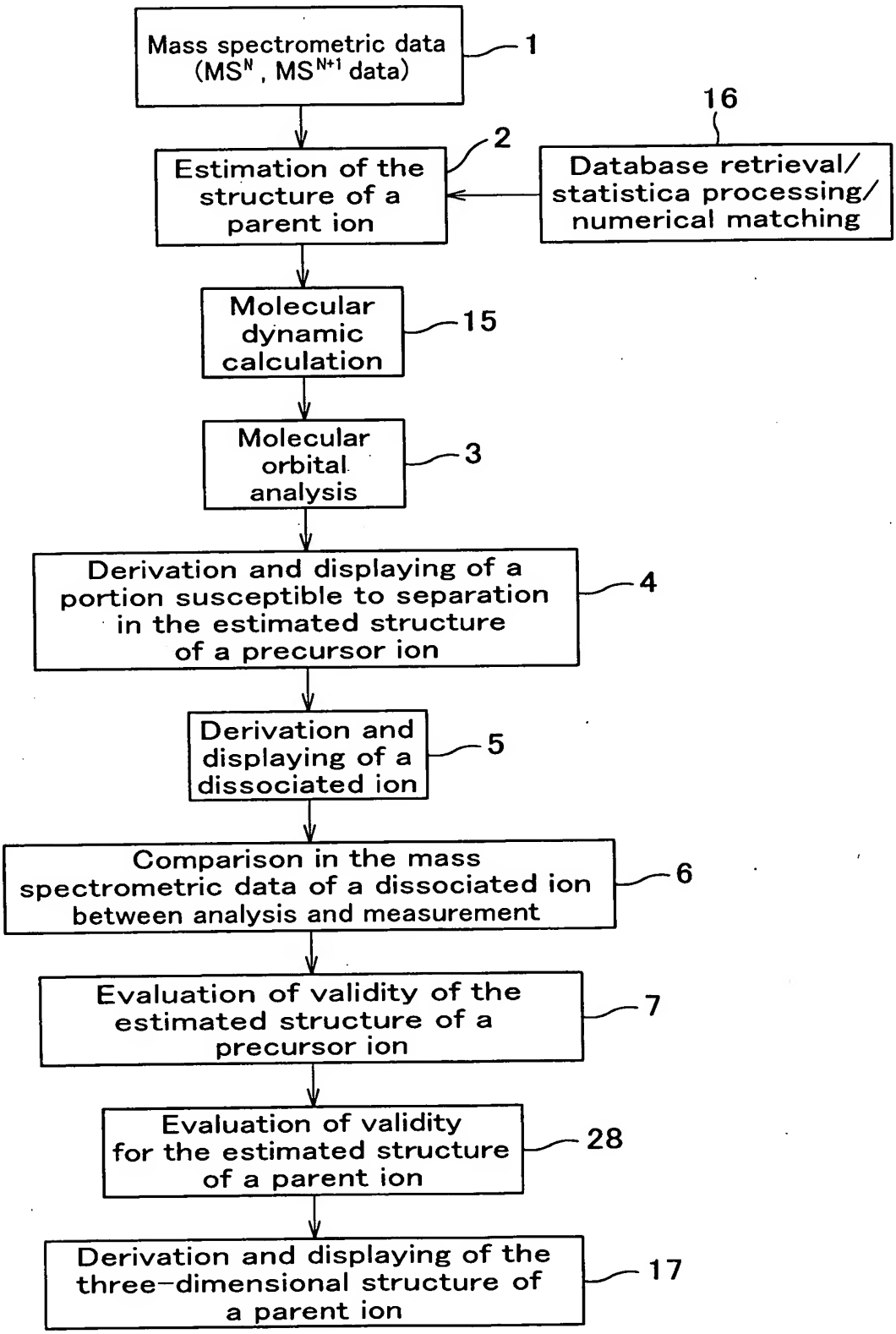

Mass spectrometric data (MS^N, MS^{N+1} data)
1
16
Estimation of the structure of a parent ion
2
Database retrieval/ statistica processing/ numerical matching
Molecular dynamic calculation
15
Molecular orbital analysis
3
Derivation and displaying of a portion susceptible to separation in the estimated structure of a precursor ion
4
Derivation and displaying of a dissociated ion
5
Comparison in the mass spectrometric data of a dissociated ion between analysis and measurement
6
Evaluation of validity of the estimated structure of a precursor ion
7
Evaluation of validity for the estimated structure of a parent ion
28
Derivation and displaying of the three-dimensional structure of a parent ion
17

FIG. 5

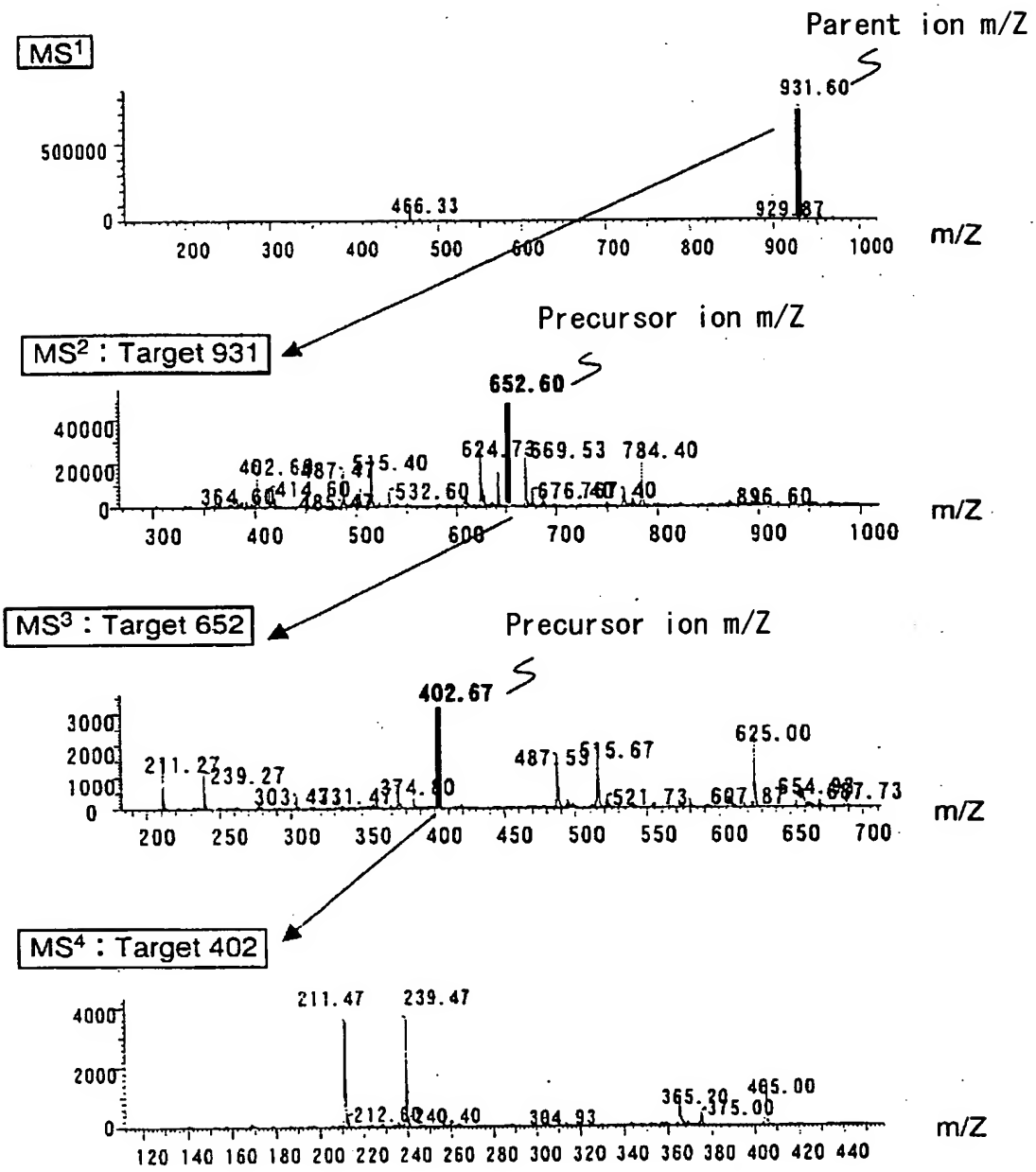

Parent ion m/Z
MS1
931.60
500000
0
466.33
929.87
200
300
400
500
600
700
800
900
1000
m/Z
Precursor ion m/Z
MS2 : Target 931
652.60
40000
20000
0
402.67
487.47
515.40
624.73
669.53
784.40
364.60
414.60
485.47
532.60
676.73
896.60
300
400
500
600
700
800
900
1000
m/Z
MS3 : Target 652
Precursor ion m/Z
402.67
3000
2000
1000
0
211.27
239.27
303.47
331.47
374.80
487.53
515.67
521.73
625.00
697.87
654.87
697.73
200
250
300
350
400
450
500
550
600
650
700
m/Z
MS4 : Target 402
211.47
239.47
4000
2000
0
212.80
240.40
304.93
365.20
375.00
405.00
120 140 160 180 200 220 240 260 280 300 320 340 360 380 400 420 440
m/Z

FIG. 6

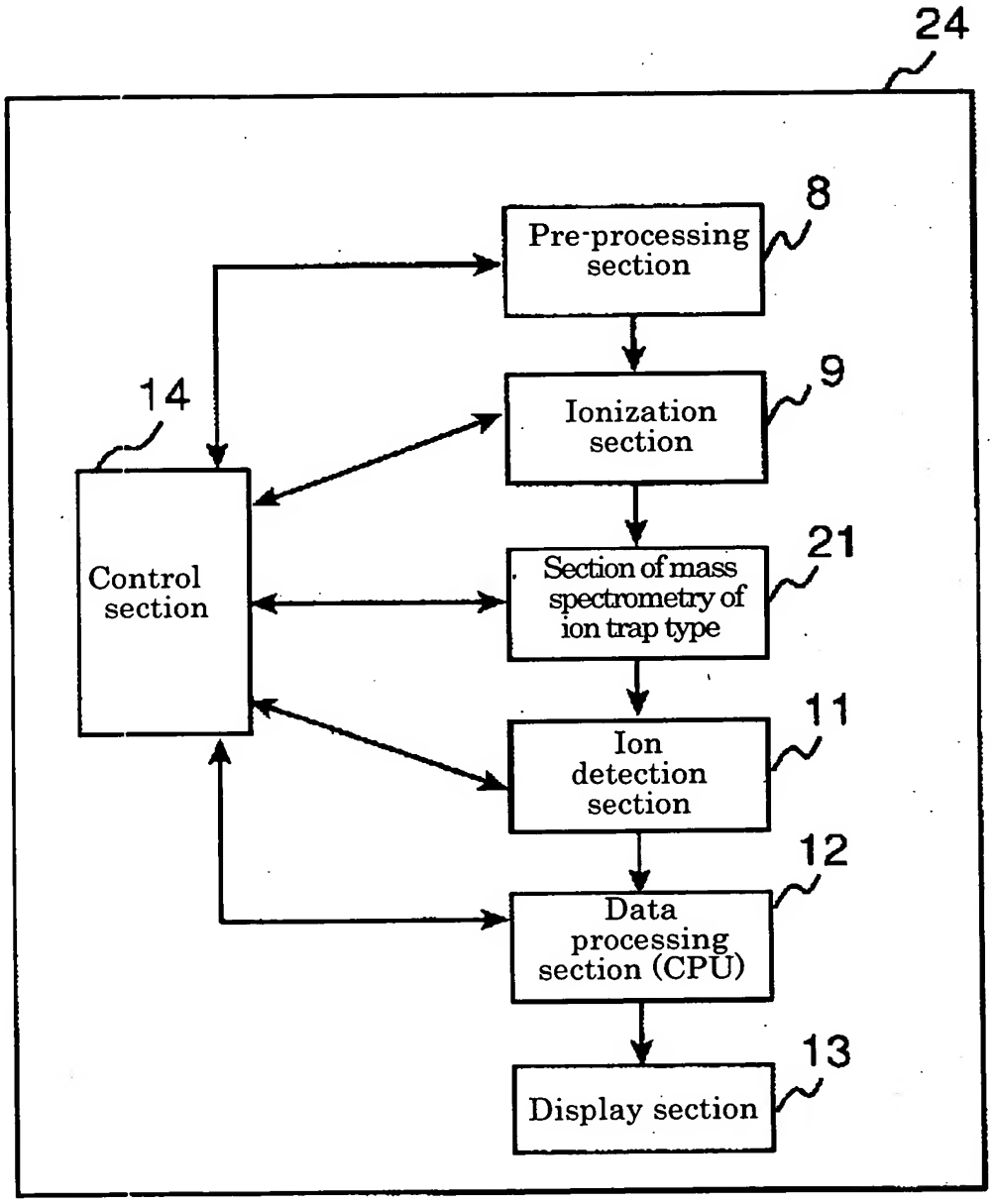
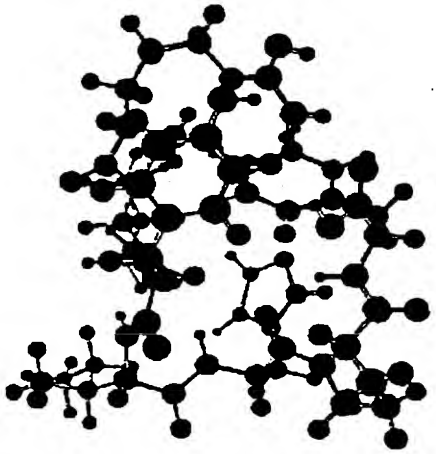

24
8
Pre-processing section
9
Ionization section
14
Control section
21
Section of mass spectrometry of ion trap type
11
Ion detection section
12
Data processing section (CPU)
13
Display section

FIG. 7

Rank	Estimated amino acid sequences (N-terminal← →C-terminal)						
1	Arg	Tyr	Val	Leu	His	Met	Leu
2	Arg	Tyr	Val	Leu	His	Met	Leu
3	Arg	Tyr	Val	Ile	His	Met	Leu
4	Arg	Tyr	Val	Leu	His	Met	Ile
5	Arg	Tyr	Val	Ile	His	Met	Ile
6	Arg	Tyr	Val	Ile	His	Met	Ile
7	Arg	Val	Tyr	Ile	His	Met	Leu
8	Arg	Val	Tyr	Leu	His	Met	Ile
9	Arg	Val	Tyr	Leu	His	Met	Leu
10	Arg	Val	Tyr	Leu	His	Met	Leu
11	Arg	Val	Tyr	Ile	His	Met	Ile
12	Arg	Val	Tyr	Ile	His	Met	Ile
13	Arg	Tyr	Val	Leu	His	Asp	Glu
14	Arg	Tyr	Val	Ile	His	Asp	Glu
15	Arg	Tyr	Val	Leu	His	Pro	Phe
16	Arg	Tyr	Val	Ile	His	Pro	Phe
17	Arg	Val	Tyr	Leu	His	Asp	Glu
18	Arg	Val	Tyr	Ile	His	Asp	Glu
19	Arg	Val	Tyr	Leu	His	Pro	Phe
20	Arg	Val	Tyr	Ile	His	Pro	Phe

FIG. 8

Rank	Estimated amino acid sequences (N-terminal← →C-terminal)							Ranking resulting from the method of invention
1	Arg	Tyr	Val	Leu	His	Met	Leu	6
2	Arg	Tyr	Val	Leu	His	Met	Leu	7
3	Arg	Tyr	Val	Ile	His	Met	Leu	13
4	Arg	Tyr	Val	Leu	His	Met	Ile	8
5	Arg	Tyr	Val	Ile	His	Met	Ile	19
6	Arg	Tyr	Val	Ile	His	Met	Ile	20
7	Arg	Val	Tyr	Ile	His	Met	Leu	12
8	Arg	Val	Tyr	Leu	His	Met	Ile	5
9	Arg	Val	Tyr	Leu	His	Met	Leu	3
10	Arg	Val	Tyr	Leu	His	Met	Leu	4
11	Arg	Val	Tyr	Ile	His	Met	Ile	17
12	Arg	Val	Tyr	Ile	His	Met	Ile	18
13	Arg	Tyr	Val	Leu	His	Asp	Glu	16
14	Arg	Tyr	Val	Ile	His	Asp	Glu	14
15	Arg	Tyr	Val	Leu	His	Pro	Phe	10
16	Arg	Tyr	Val	Ile	His	Pro	Phe	2
17	Arg	Val	Tyr	Leu	His	Asp	Glu	15
18	Arg	Val	Tyr	Ile	His	Asp	Glu	11
19	Arg	Val	Tyr	Leu	His	Pro	Phe	9
20	Arg	Val	Tyr	Ile	His	Pro	Phe	1



17

Arg-Val-Tyr-Ile-His-Pro-Phe

FIG. 9

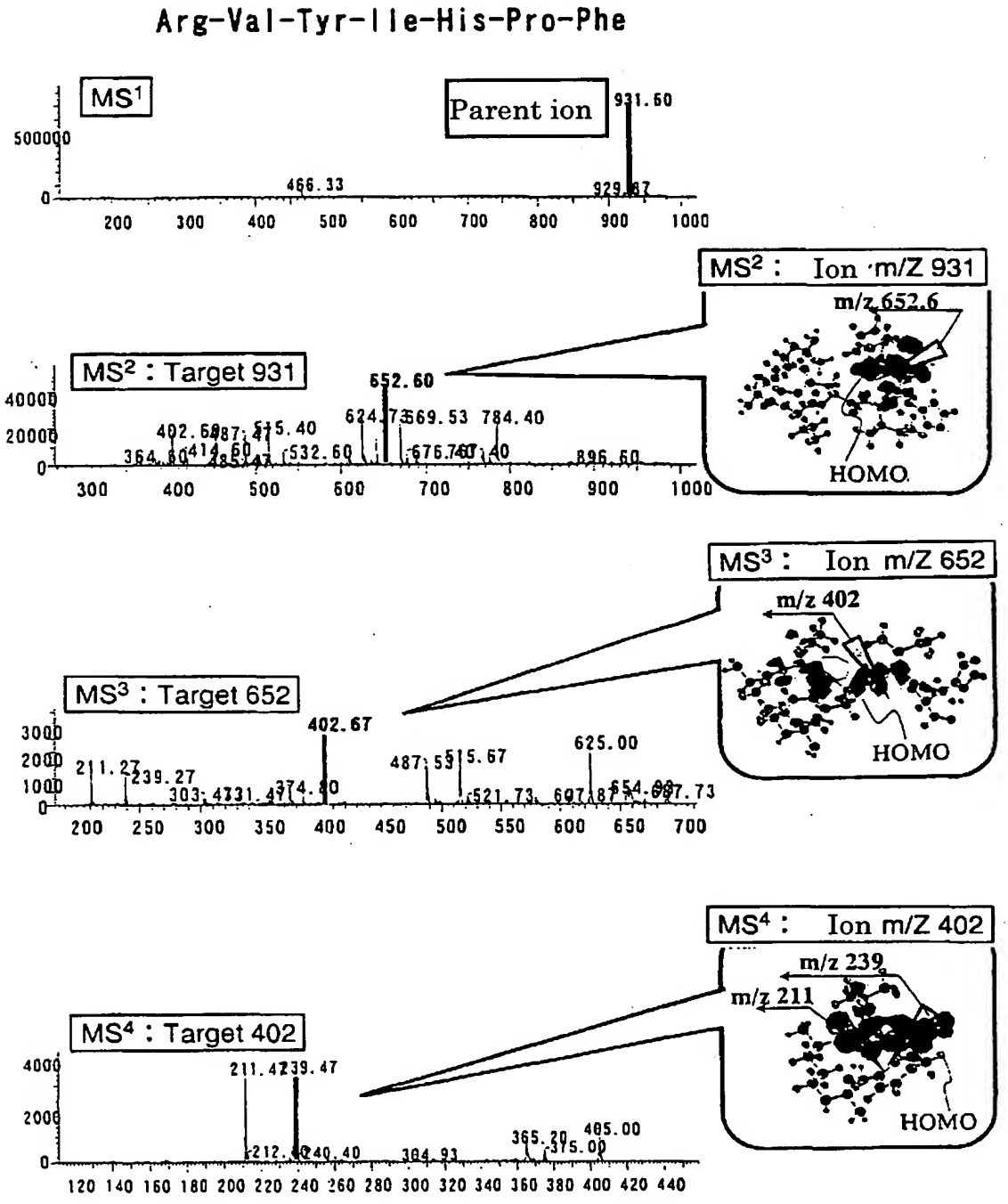
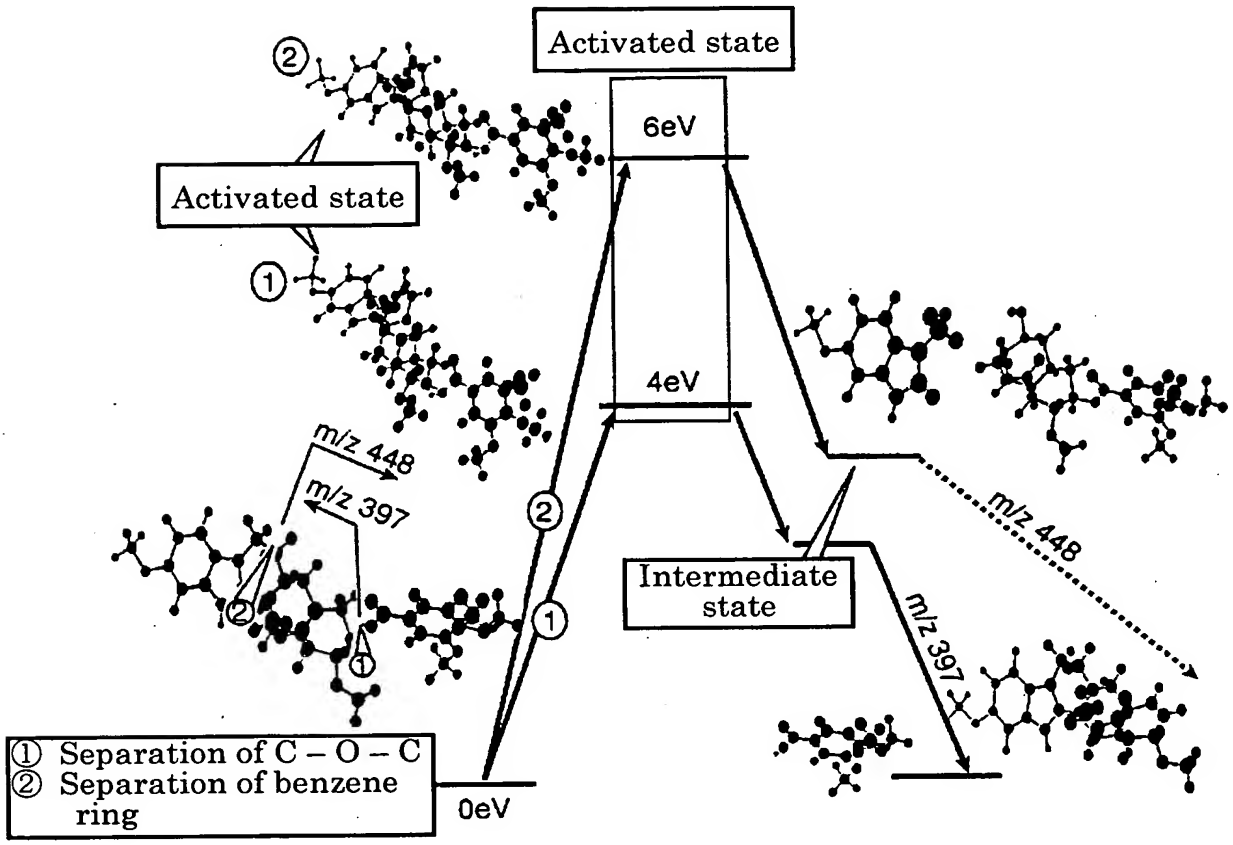

Arg-Val-Tyr-Ile-His-Pro-Phe
MS1
Parent ion
931.60
466.33
MS2 : Target 931
652.60
MS2 : Ion m/Z 931
m/z 652.6
HOMO
MS3 : Target 652
402.67
MS3 : Ion m/Z 652
m/z 402
HOMO
MS4 : Target 402
211.42
239.47
MS4 : Ion m/Z 402
m/z 239
m/z 211
HOMO

FIG. 10



DECOMPOSING REACTION OF RECERPINE

FIG. 11

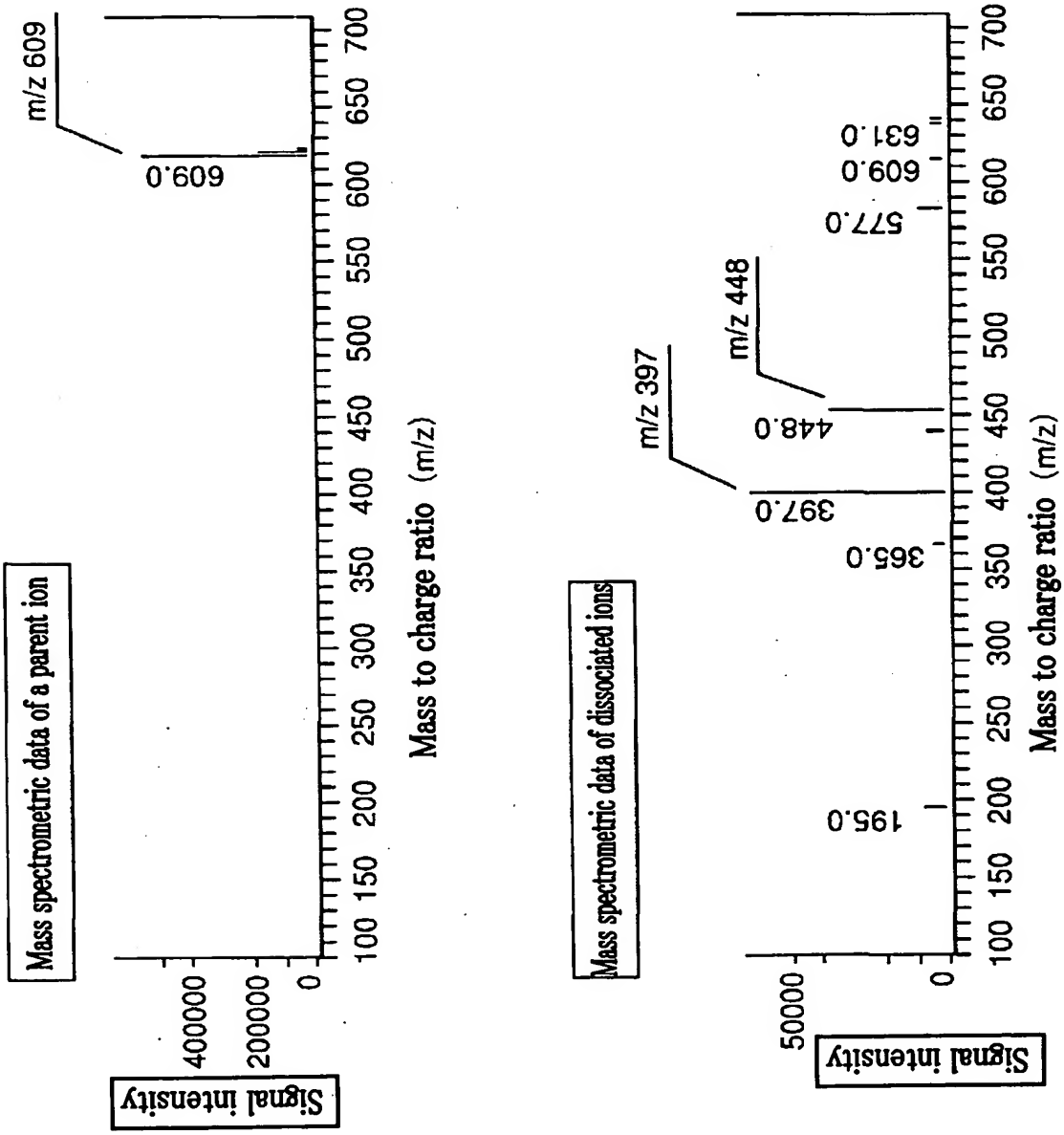

Mass spectrometric data of a parent ion
Signal intensity
0
200000
400000
100 150 200 250 300 350 400 450 500 550 600 650 700
Mass to charge ratio (m/z)
609.0
m/z 609
Mass spectrometric data of dissociated ions
Signal intensity
0
50000
100 150 200 250 300 350 400 450 500 550 600 650 700
Mass to charge ratio (m/z)
195.0
365.0
397.0
448.0
577.0
609.0
631.0
m/z 397
m/z 448

FIG. 12

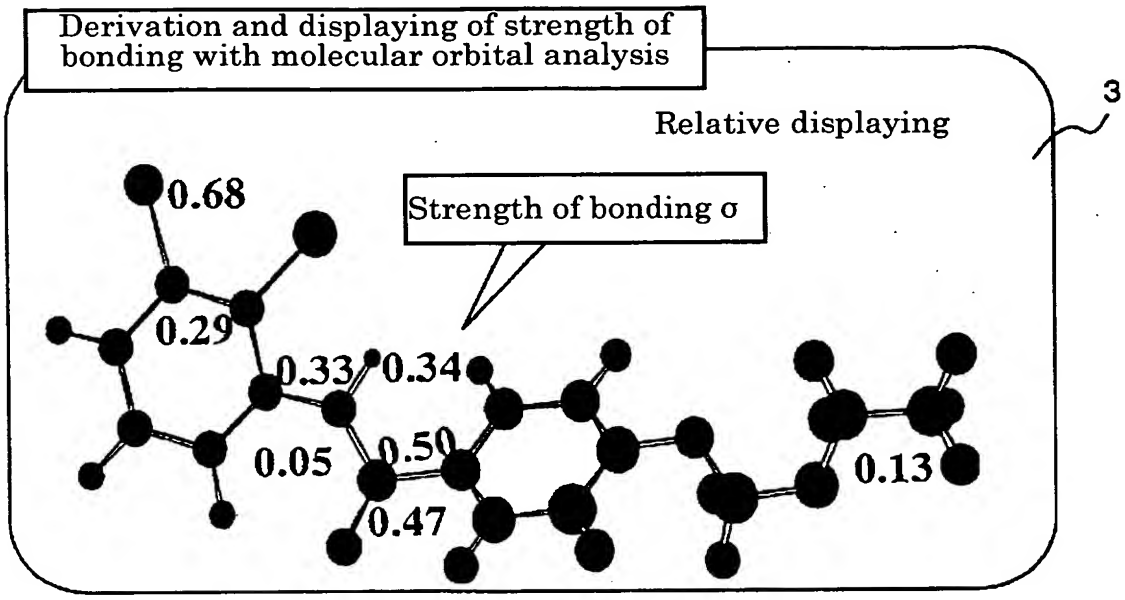

Derivation and displaying of strength of bonding with molecular orbital analysis
Relative displaying
3
Strength of bonding σ
0.68
0.29
0.33
0.34
0.05
0.50
0.47
0.13

FIG. 13

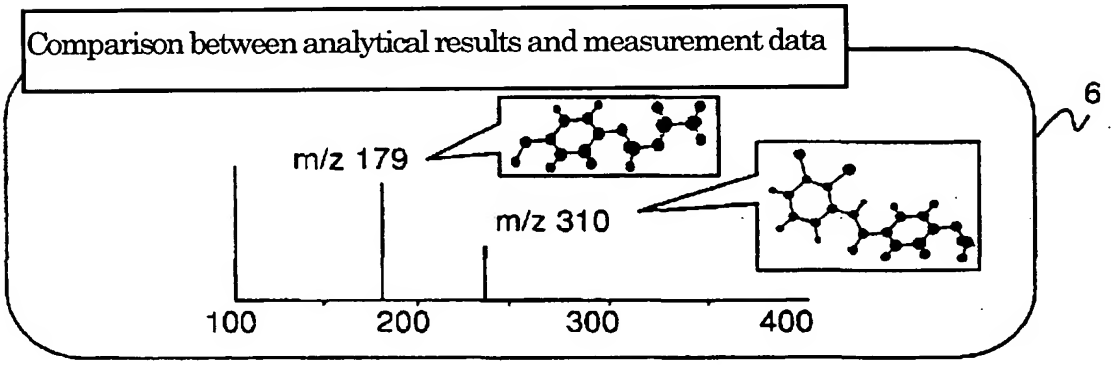

Comparison between analytical results and measurement data
6
m/z 179
m/z 310
100
200
300
400

FIG. 14

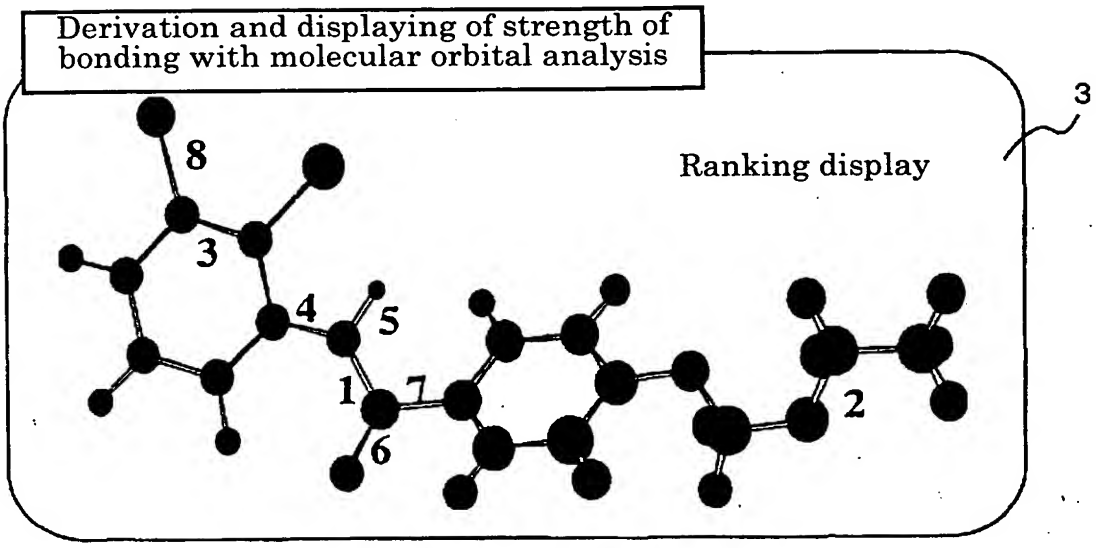

Derivation and displaying of strength of bonding with molecular orbital analysis
Ranking display
3
8
3
4
5
1
7
6
2

FIG. 15

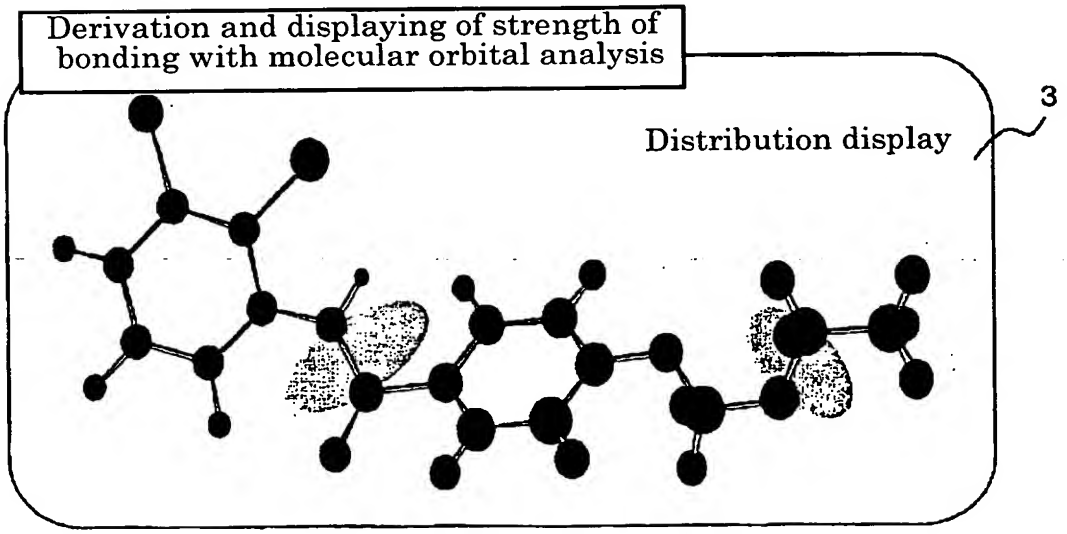

Derivation and displaying of strength of bonding with molecular orbital analysis
Distribution display
3

FIG. 16

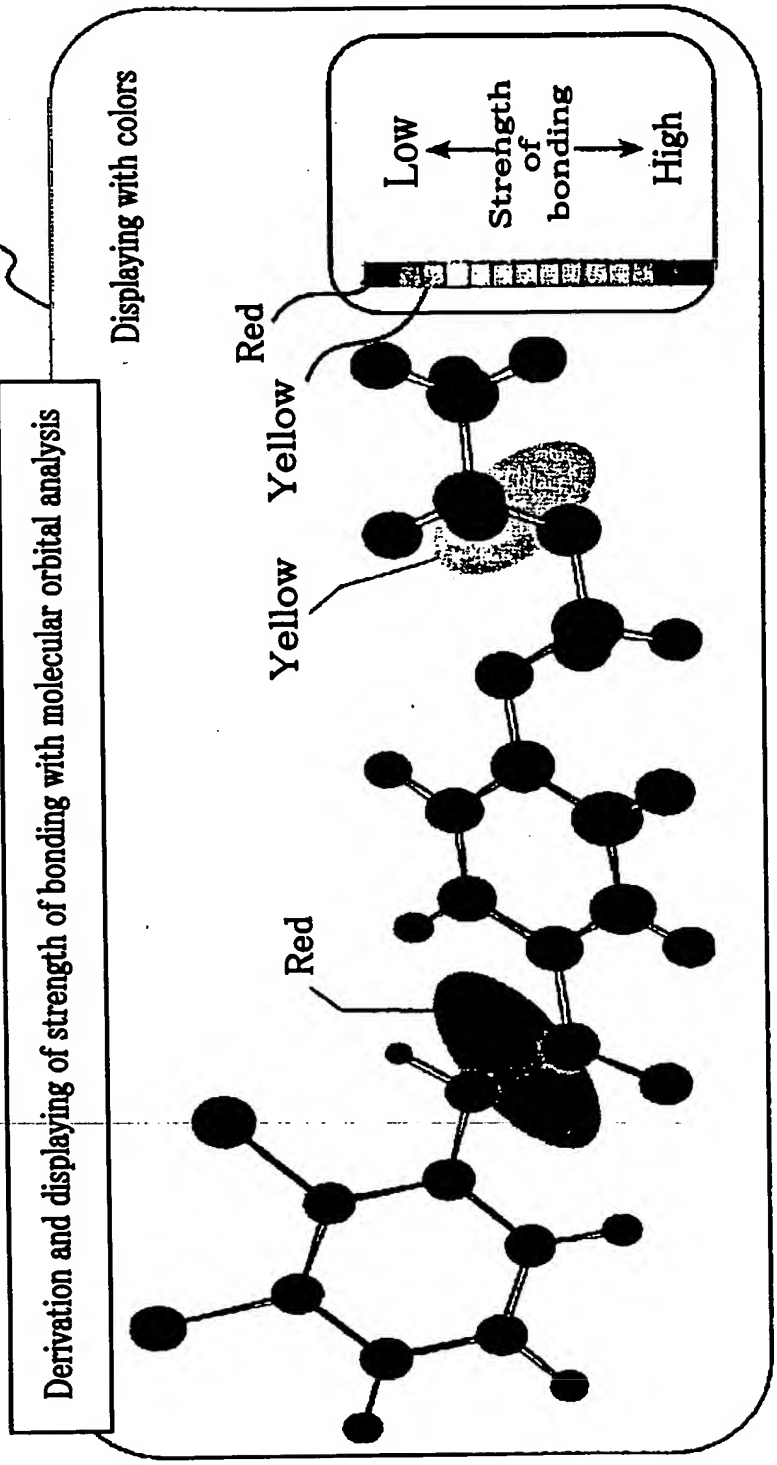

3
Derivation and displaying of strength of bonding with molecular orbital analysis
Displaying with colors
Low
Strength of bonding
High
Red
Yellow
Yellow
Red

FIG. 17

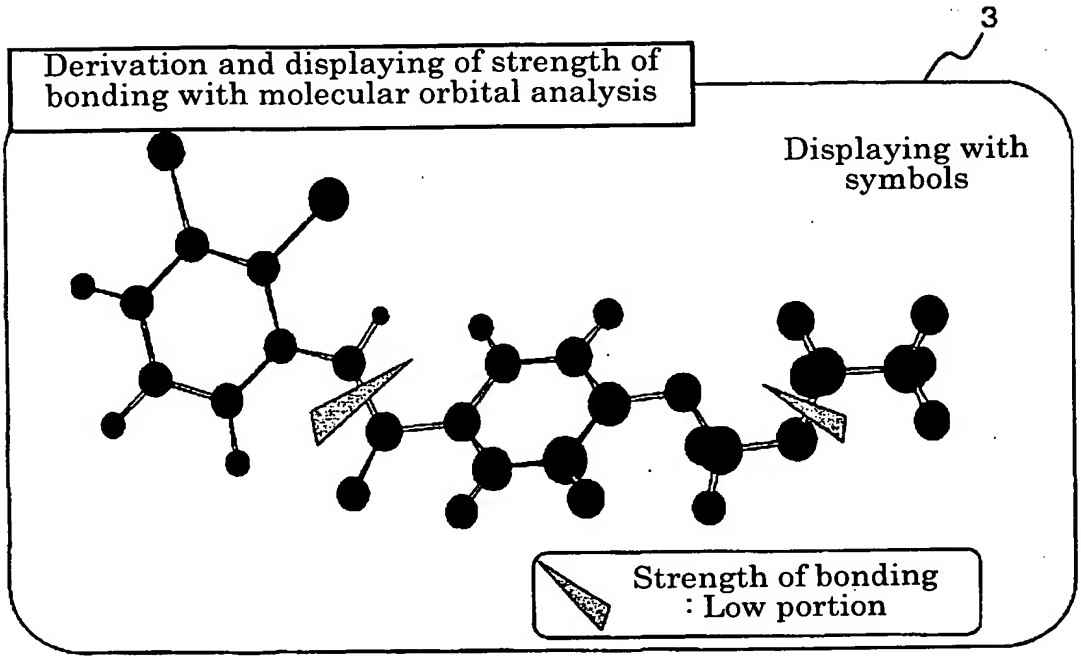

3
Derivation and displaying of strength of bonding with molecular orbital analysis
Displaying with symbols
Strength of bonding
: Low portion

FIG. 18

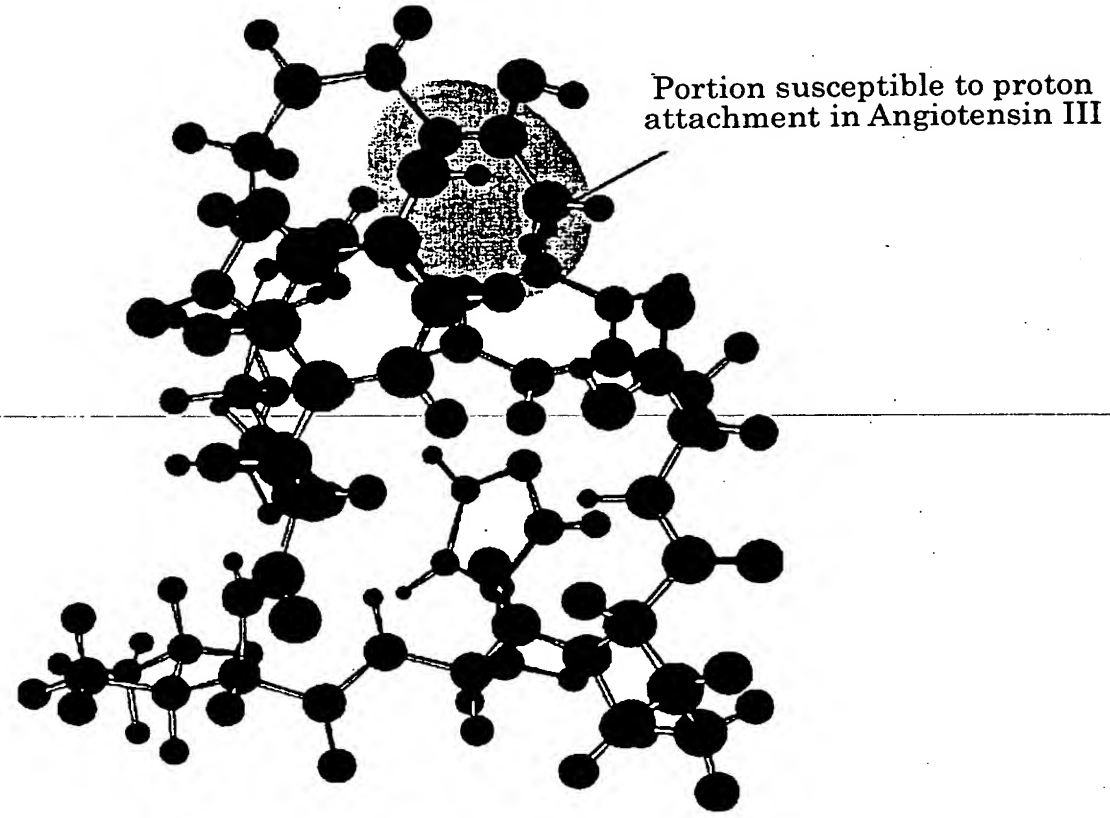

Portion susceptible to proton attachment in Angiotensin III
Arg-Val-Tyr-Ile-His-Pro-Phe

FIG. 19

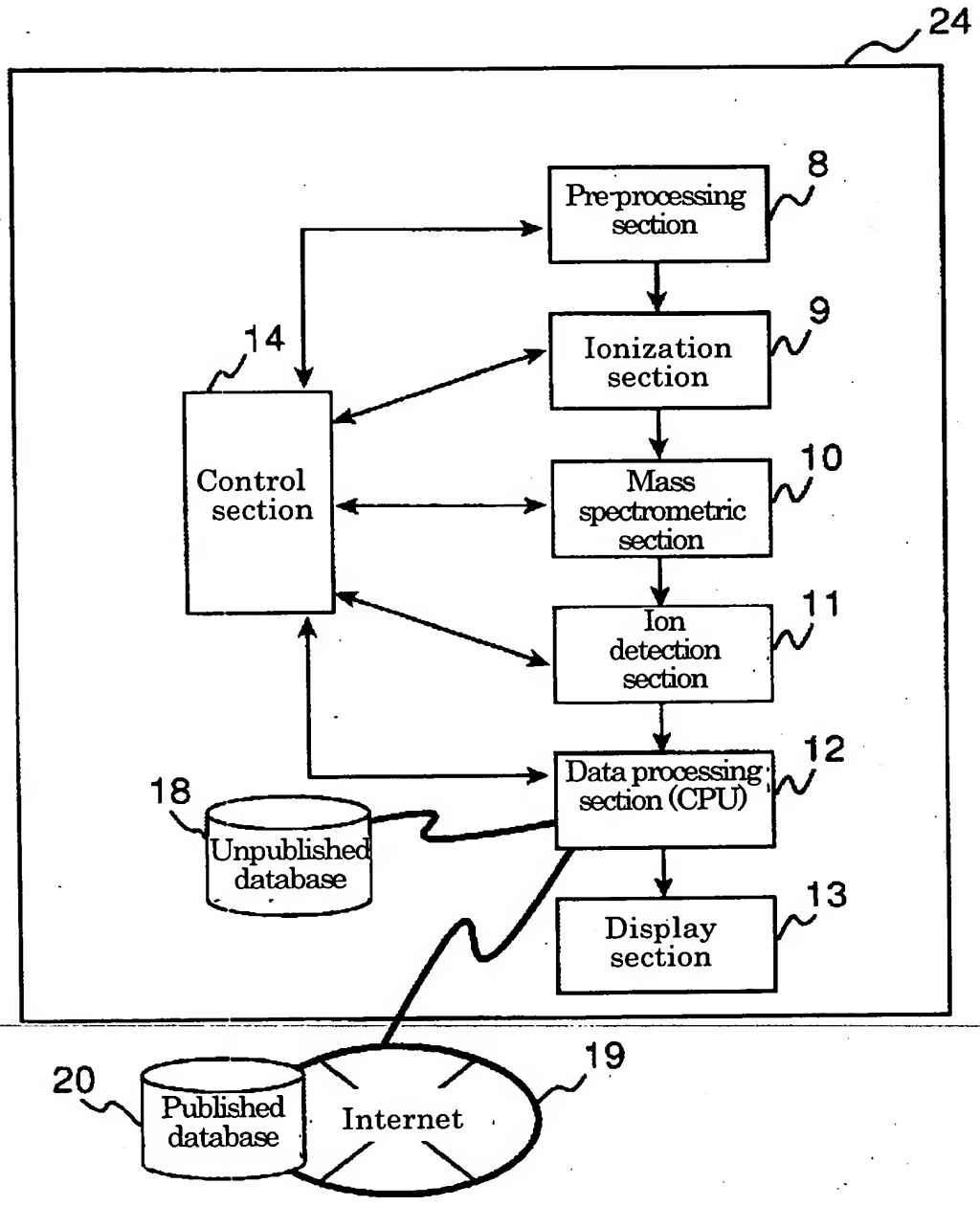
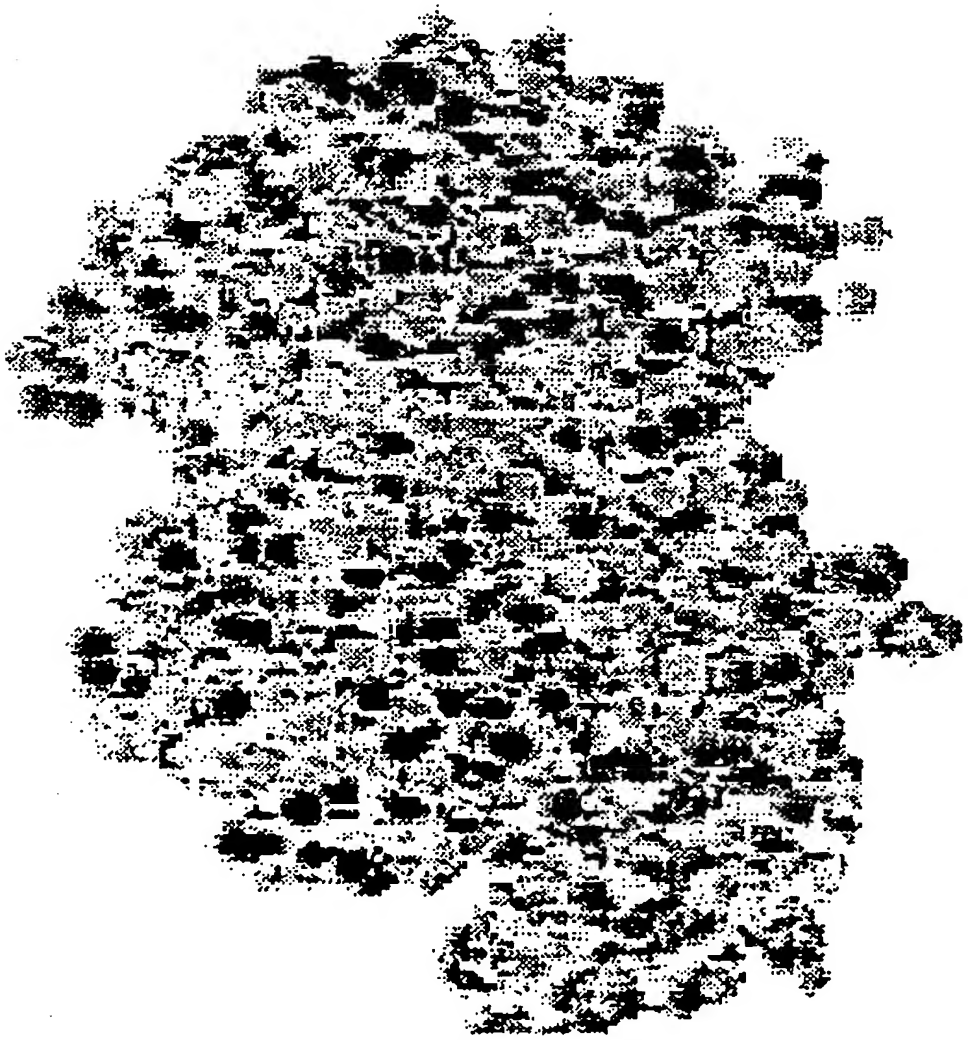

24
Pre-processing section
8
Ionization section
9
14
Control section
Mass spectrometric section
10
Ion detection section
11
Data processing section (CPU)
12
18
Unpublished database
Display section
13
20
Published database
Internet
19

FIG. 20



Three-dimensional displaying of the structure of a protein including the predicted amino acid sequence

FIG.21

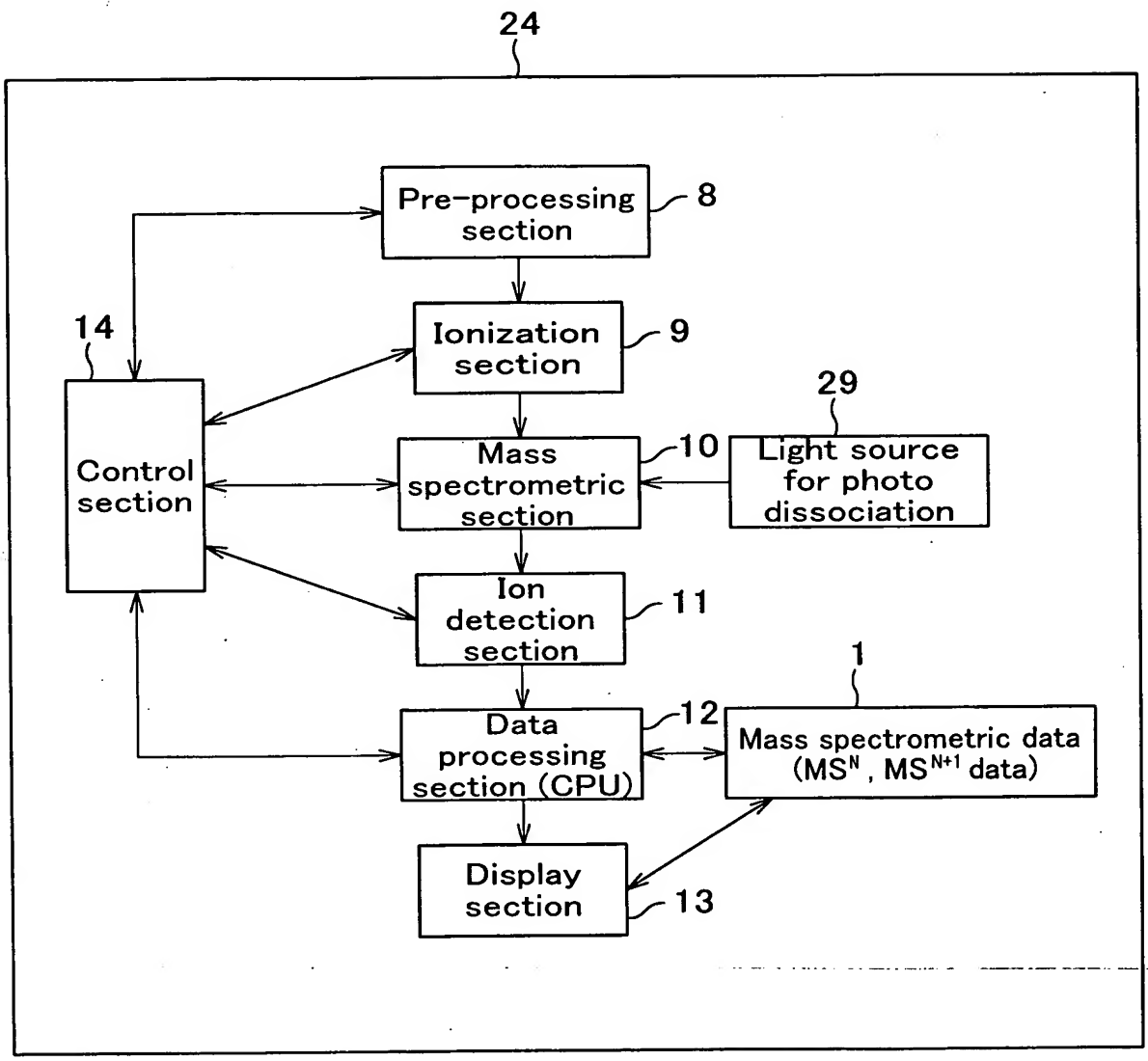

24
Pre-processing section
8
Ionization section
9
14
Control section
29
Mass spectrometric section
10
Light source for photo dissociation
Ion detection section
11
1
Data processing section (CPU)
12
Mass spectrometric data (MS^N, MS^N+1 data)
Display section
13

FIG.22

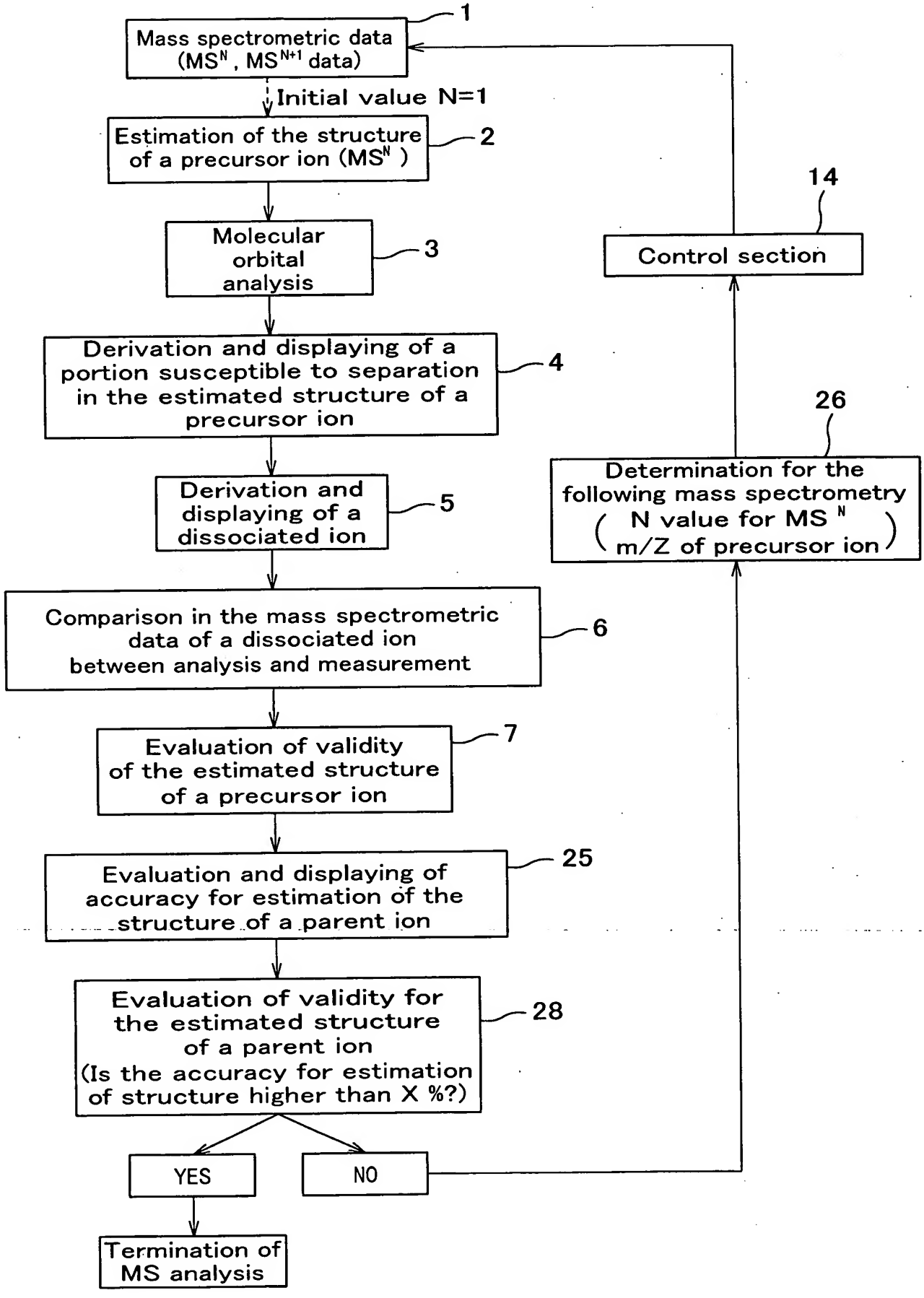

1
Mass spectrometric data (MS^N, MS^N+1 data)
Initial value N=1
Estimation of the structure of a precursor ion (MS^N)
2
Molecular orbital analysis
3
Derivation and displaying of a portion susceptible to separation in the estimated structure of a precursor ion
4
Derivation and displaying of a dissociated ion
5
Comparison in the mass spectrometric data of a dissociated ion between analysis and measurement
6
Evaluation of validity of the estimated structure of a precursor ion
7
Evaluation and displaying of accuracy for estimation of the structure of a parent ion
25
Evaluation of validity for the estimated structure of a parent ion (Is the accuracy for estimation of structure higher than X %?)
28
YES
NO
Termination of MS analysis
14
Control section
26
Determination for the following mass spectrometry (N value for MS^N m/Z of precursor ion)

FIG. 23

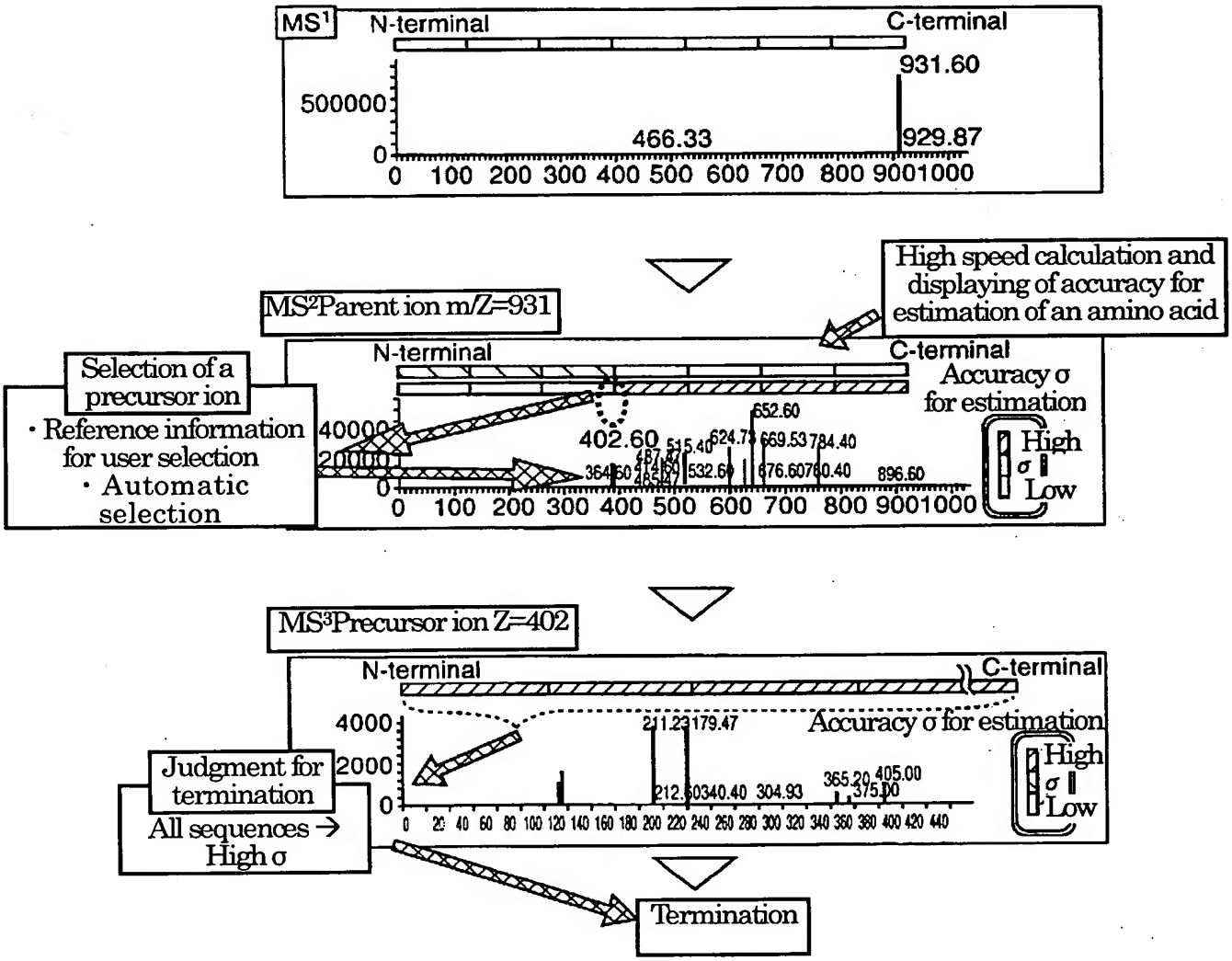

MS1
N-terminal
C-terminal
931.60
500000
466.33
929.87
0
0 100 200 300 400 500 600 700 800 9001000
High speed calculation and displaying of accuracy for estimation of an amino acid
MS2Parent ion m/Z=931
Selection of a precursor ion
・Reference information for user selection
・Automatic selection
N-terminal
C-terminal
Accuracy σ for estimation
40000
20000
0
402.60
652.60
High
σ
Low
MS3Precursor ion Z=402
N-terminal
C-terminal
4000
2000
0
211.23
179.47
Accuracy σ for estimation
Judgment for termination
All sequences → High σ
Termination

FIG. 24

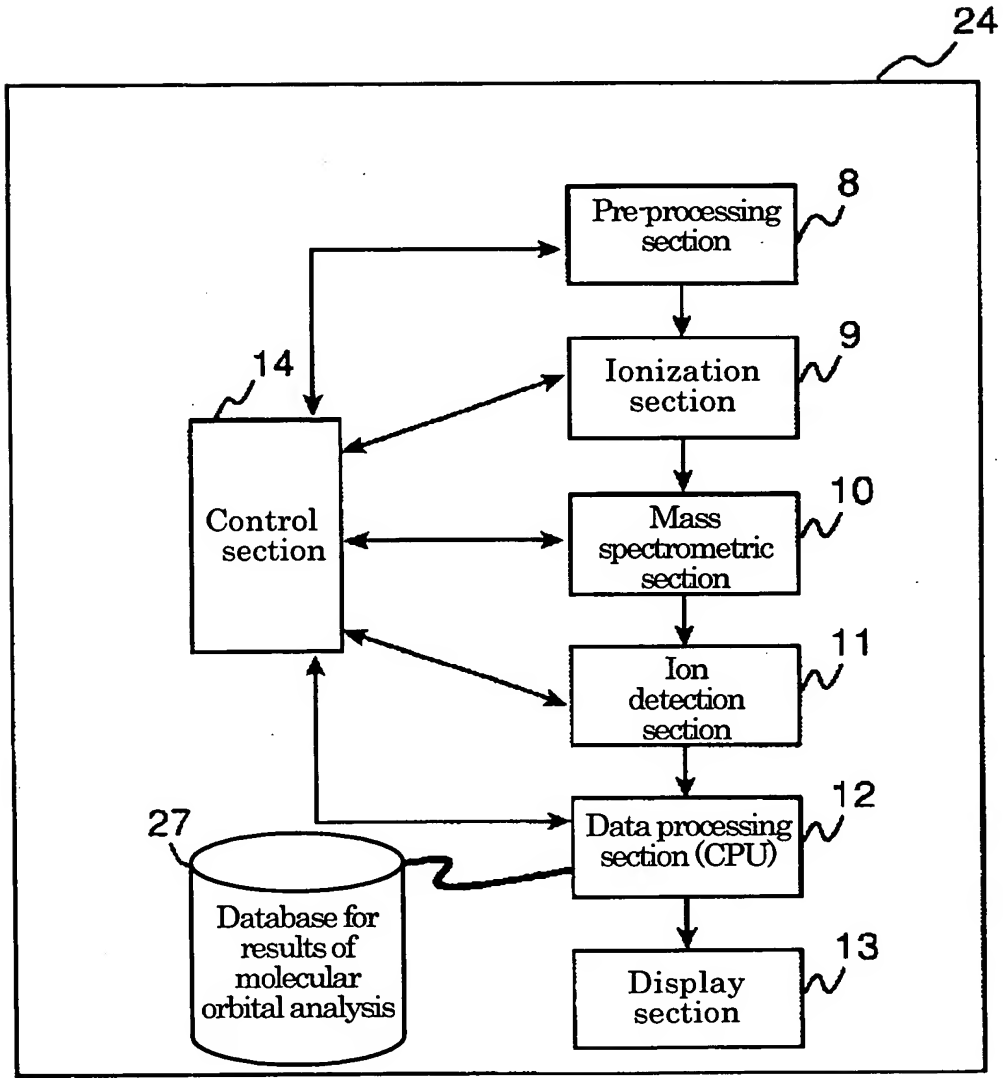

24
Pre-processing section
8
Ionization section
9
14
Control section
Mass spectrometric section
10
Ion detection section
11
27
Data processing section (CPU)
12
Database for results of molecular orbital analysis
Display section
13

FIG.25

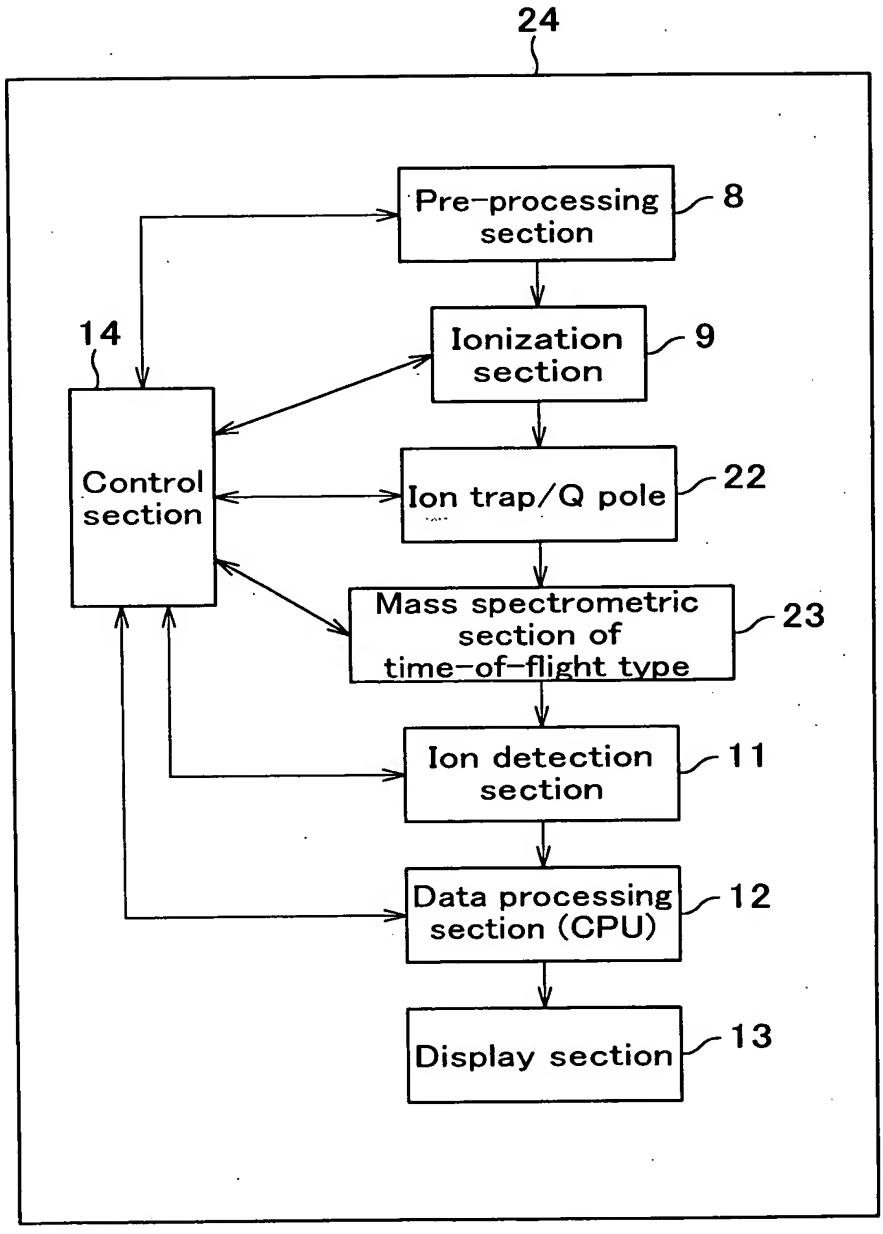

24
Pre-processing section
8
Ionization section
9
14
Control section
Ion trap/Q pole
22
Mass spectrometric section of time-of-flight type
23
Ion detection section
11
Data processing section (CPU)
12
Display section
13

FIG.26

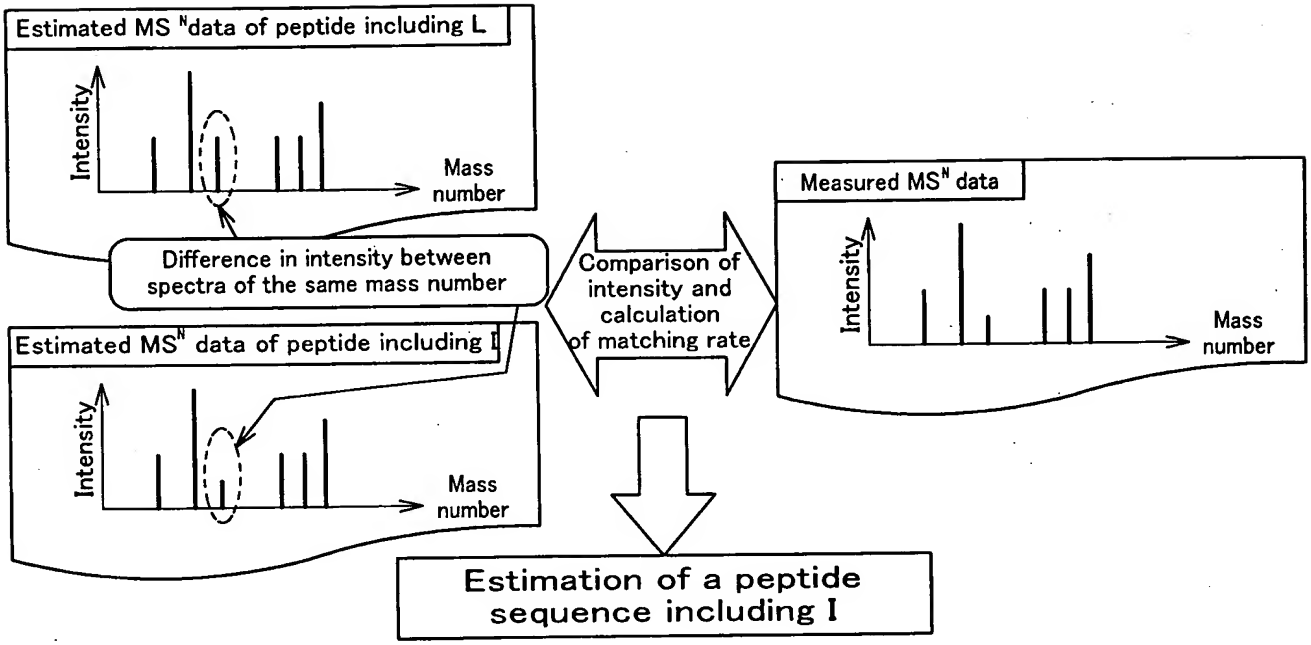

Estimated MS Ndata of peptide including L
Intensity
Mass number
Difference in intensity between spectra of the same mass number
Estimated MS^N data of peptide including I
Intensity
Mass number
Comparison of intensity and calculation of matching rate
Measured MS^N data
Intensity
Mass number
Estimation of a peptide sequence including I

FIG. 27

Combination of a single amino acid and a pair of amino acids having the same or close mass number

1 Single amino acid	2 A pair of amino acids	Difference of mass number
Trp (186.213) ,	Glu-Gly (186168)	Δm=0.0458
Trp (186.213) ,	Ala-Asp (186.168)	Δm=0.0458
Trp (186.213) ,	Ser-Val (186.211)	Δm=0.0024
Trp (186.213) ,	Lys-Gly (185.226)	Δm=0.9872
Trp (186.213) ,	Gln-Gly (185.183)	Δm=1.0305
Trp (186.213) ,	Asn-Ala (185.183)	Δm=1.0305
Asn (114.104) ,	Gly-Gly (114.104)	Δm=0
Lys (128.174) ,	Gly-Ala (128.131)	Δm=0.0434
Gln (128.131) ,	Gly-Ala (128.131)	Δm=0
Arg (156.188) ,	Val-Gly (156.185)	Δm=0.0031
Glu (129.116) ,	Gly-Ala (128.131)	Δm=0.9847

$|\Delta m| < 1.0$

( ):Mass number without N and C terminals